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A rigid ion second neighbor force constant phonon model was developed for chalcopyrites with zincblende parent compound as a limiting case. Study of zincblende to chalcopyrite mappings led to development of a Brillouin zone special point summation theory. Brout's sum rule was shown to be a limiting case of this theory.
The importance of the relation between zincblende and chalcopyrite phonon deformation parameters led to development of a phenomenological model for → next page

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zincblende phonon deformation model valid throughout the Brillouin zone. The techniques developed for generating this model are simpler than others published to date and are applicable to any symmetry based model.

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Final Report on Contract N00014-76-C-0384

Investigation on Chalcopyrite Semiconductors

George B. Wright
May, 1978

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The work on this contract was directed to investigation of problems associated with Chalcopyrite and related tetrahedrally coordinated ternary semiconductor compounds. The chalcopyrites are of interest not only because of their intrinsic optical and electronic properties, but also because of their close structural relation to the better known classical semiconductors, the diamond and zincblende types exemplified for example by silicon and gallium arsenide.

As a starting point for the work on this contract, we investigated the symmetry relation between chalcopyrites and zincblende. The cubic zincblende structure consists of two interpenetrating face-centered cubic (FCC) sublattices. The chalcopyrite structure has eight body-centered tetragonal (BCT) sublattices. Taking the lattice vibrational problem as a vehicle to study the general properties, we developed a model for transition between zincblende and chalcopyrite phonons which introduced the equivalent of structure factors into the dynamical secular equation for phonons. The structure factors disappear for the zincblende model and leave one at a general q-point in the Brillouin Zone (BZ) with a factored secular equation mapping into four q-points of the zincblende BZ. The 4-fold mapping was previously known, but in deeper investigation of its significance, we were led to a more general formulation of the mapping problem. We were able to apply group theory to a generalization of Brout's Sum Rule for phonons. This sum rule, widely used for phonon spectral investigations in the 1960's, states that the sum of phonon frequencies squared at a given point in the BZ is roughly constant. We showed that Brout's Sum Rule is the first term in a hierarchy of sum rules, and that the accuracy is related to the "range" of force constants involved. A deeper investigation of this problem led to a generalization of a number of treatments of the "Special Point" problem in the BZ. The first definition of a "special point" was given by Baldereschi, who pointed out that in taking averages of periodic quantities over the BZ,

it was possible to choose one mean value point in the BZ, which depends only on the translational symmetry of the crystal. This approximation was refined by other workers in later papers. We have found the underlying mechanism for these results and completely generalised them in a geometric model involving factor groups. Work is still in progress on this question.

An experimental investigation of Cu_3PS_4, a related tetrahedral compound with orthorhombic symmetry was published in the Proceedings of the Semiconductor Conference at Rome*. In a master's thesis investigation by Mr. V. Garcia, a phonon model was developed for zincblende chalcopyrites, which matched experimental data as well or better than published results. Nevertheless, we found that variation of first neighbor force constants did not lead to a correct sequence of symmetry types for low frequency phonons. A similar problem has been observed in published results. Realising the importance that Gruneissen effects on phonon frequency shifts under applied strain would have in shedding light on chalcopyrite problems we started a formulation of strain effects on phonons throughout the B. Z. Our first model for phonons in diamond structures, based on the valence force field approach, lead to a model in which only nine parameters give the phonon dispersion relations throughout the BZ within experimental accuracy of neutron scattering spectroscopy for diamond silicon germanium and gray tin. Presently we have been developing a general formulation for strain effects on the phonon dispersions relations throughout the zone. We have developed a new group-theoretical technique for use on the problem which promises to lend itself well to computer automation. Work is still in progress on this problem. Papers are in preparation for publication of the results on Brout's sum rule, the generalized mapping formulation, thermal expansion theory in chalcopyrites, and the phonon-strain problem.

George B. Wright
May, 1978